

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 |

Model Results

Predicted value: 118 °C

Global applicability domain: Inside

Local applicability domain index: 7.87e-01

Confidence level: 8.14e-01

Nearest Neighbors from the Training Set

[Image not found](#)

But-2-en-1-ol

Measured: 121

Predicted: 118

[Image not found](#)

3-Buten-1-ol

Measured: 114

Predicted: 114

[Image not found](#)

Cyclobutanol

Measured: 124

Predicted: 120

[Image not found](#)

2-Methoxy-1-propanol

Measured: 130

Predicted: 129